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Solid-Solid Phase Transitions of Rare Gases in Cylindrical Pores

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Introduction: It is well known that confinement and finite-size can cause changes in the thermodynamic properties of materials. Depression of the freezing transition, changes in structure, and induced phase transitions are just a few of these interesting results. The data presented here focus on the introduction of solid-solid phase transitions in rare gases induced by confinement.

Rare gases are typically chosen for study as a result of their simple phase diagram. They will crystallize into an fcc structure on freezing with no further transitions to 0K. Recent studies have shown that confinement causes significant change to this simple phase diagram. Brown, *et al*. performed studies on Ar and Kr confined in a monolithic Vycor sample [1]. Not only did the rare gases crystallize into a dhcp structure on freezing, they discovered a solid-solid transition that occurs at about half the melting temperature, where fcc crystallites form in coexistence with the dhcp powder. More recently, Silva *et al*. performed measurements of Ar and Kr confined in powdered sol-gel and Vycor [2]. They also saw the Ar and Kr crystallize into a dhcp structure on freezing, but saw an entirely new solid-solid phase transition. The solid developed a high mobility and migrated out of the pore space.

Methods and Materials: X-ray diffraction studies were performed on samples of Ar and Kr confined in the porous glasses, MCM-41 and SBA-15. Both of these glasses have a hexagonal array of 1-D pores. The only difference would be that the SBA-15 was treated to remove micropores. All samples were filled to 100% in the solid.

Results: All results for both the Ar and Kr confined in the MCM and SBA samples are very similar. Therefore, we will present the results for Ar confined in a 60Å sample of SBA-15, shown in figure 1. As in the previous measurements, the Ar has a liquid-like component similar to that of the bulk, as seen in the 85K measurement. The Ar also crystallizes into a dhcp structure on freezing as seen at 65K. A solid-solid phase transition also exists that occurs at $T \sim 0.70T_m$. Much like the results of Brown, *et al*., very sharp diffraction peaks appear that can be indexed as fcc. However, the overall scattering decreases as seen by the less intense dhcp peaks and amorphous peak.

Conclusions: The results show an increase in mobility of the rare gases. This higher mobility causes a transition to the energetically more favorable fcc structure. However, it also results in the loss of the amorphous component (the rare gas adsorbed on the pore walls), which should not happen if the structure was only making a transition from the dhcp to the fcc. It would appear that a fraction of the rare gas is leaving the pores. This increased mobility is much larger than typical diffusion of a solid, but less than that seen by Silva, *et al*. when confined in powdered sol-gel and Vycor.

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References: [1] Brown, *et al*. Phys. Rev. Lett. **81**, 1019 (1998). [2] Silva, *et al*. Phys. Rev. Lett. **88**, 155701-1 (2002).

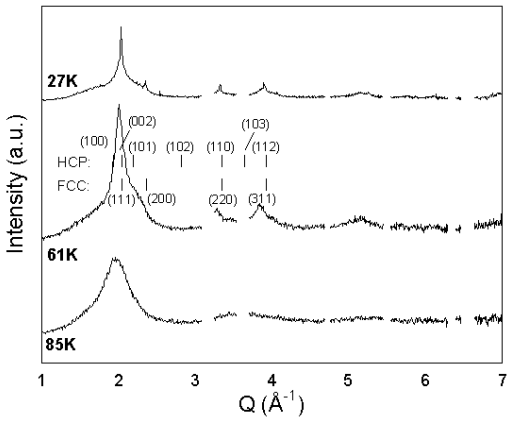

Figure 1. Diffraction measurement of Argon confined in a 60Å sample with Be peaks removed and attenuation accounted for. Note the appearance of the sharp fcc reflections at the lowest temperature.